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L1	786	(514/301,546/114).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/12/12 11:12
L2	23	I1 and selectin	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/12/12 11:12

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PASSWORD:

* , = * * ·

TERMINAL (ENTER 1, 2, 3, OR ?):2

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         JUL 02
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         JUL 02
                 SCISEARCH enhanced with complete author names
         JUL 02
NEWS
                 CHEMCATS accession numbers revised
         JUL 02
                 CA/CAplus enhanced with utility model patents from China
NEWS
         JUL 16
NEWS
                CAplus enhanced with French and German abstracts
NEWS
         JUL 18
                 CA/CAplus patent coverage enhanced
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         JUL 26
                 USPATFULL/USPAT2 enhanced with IPC reclassification
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         JUL 30
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NEWS 10 AUG 06
                 CAS REGISTRY enhanced with new experimental property tags
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        AUG 06
                 FSTA enhanced with new thesaurus edition
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        AUG 13
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                 patents
                 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 13 AUG 20
NEWS 14
        AUG 27
                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
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                 spectral property data
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                 World Patents Index
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         SEP 13
                 FORIS renamed to SOFIS
NEWS 19
         SEP 13
                 INPADOCDB enhanced with monthly SDI frequency
NEWS 20
        SEP 17
                 CA/CAplus enhanced with printed CA page images from
                 1967-1998
NEWS 21
         SEP 17
                 CAplus coverage extended to include traditional medicine
NEWS 22
         SEP 24
                 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23
        OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS 24 OCT 19
                 BEILSTEIN updated with new compounds
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                 Derwent Indian patent publication number format enhanced
NEWS 26 NOV 19
                 WPIX enhanced with XML display format
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                 ICSD reloaded with enhancements
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                 LINPADOCDB now available on STN
             19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
NEWS EXPRESS
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(jp),
              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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FULL ESTIMATED COST

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chain nodes :

=>

10 11 12 19 21 22 23 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

ring/chain nodes :

·, ·.

chain bonds :

8-10 10-11 10-23 11-12 11-13 14-26 15-25 16-19 17-28 18-27 19-20 19-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-10 10-11 11-12 16-19 19-20 19-21 19-22

exact bonds :

5-7 6-9 7-8 8-9 10-23 11-13 14-26 15-25 17-28 18-27

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems : containing 1 : 13 :

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 11:15:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 206 TO ITERATE

100.0% PROCESSED 206 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: PROJECTED ANSWERS:

3259 TO 4981 3027 TO 4693

L2

50 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 11:15:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3831 TO ITERATE

100.0% PROCESSED 3831 ITERATIONS

3524 ANSWERS

SEARCH TIME: 00.00.01

L3 3524 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

172.10 172.31

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=> s 13 full

L4 3 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1331198 CAPLUS
DOCUMENT NUMBER: 146:184625
30 pharmacophore based virtual screening of T-type calcium channel blockers AUTHOR (S):

calcium channel blockers
Doddareddy, Munikumar Reddyr Choo, Hyunahr Cho, Yong
Seor Rhim, Hyewhon, Koh, Hun Yeongr Lee, Jung-Han
Jeong, Seong-Woor Pae, As Nim
Life Science Division, Korea Institute of Science and
Technology, Seoul, 130-650, S. Korea
Bioorganic & Medicinal Chemistry (2007), 15(2),
1091-1105

CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP: ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: LANGUAGE: English

Virtual screening of the com. databases was done by using a three dimensional pharmacophore previously developed for T-type calcium channel blockers using CATALYST program. Biol. evaluation of 25 selected virtual hits resulted in the discovery of a highly potent compound (1) with ICSO value of 0.10 µM, eight times as potent as the known selective T-type calcium channel blocker, mibefradil. Search for similar compds, yielded several hits with micro-molar ICSO values and high T-type calcium channel selectivity. Based on the structure of the virtual hits, small mol. libraries with novel scaffolds were designed, synthesis and biol. evaluation of which are currently in progress. This result shows a successful example of ligand based drug discovery of potent T-type calcium channel blockers.
449767-52-6
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USSS (Uses)
(30 pharmacophore based virtual screening of T-type calcium channel blockers)
449767-52-6 CAPIUS
Thieno[2,3-c]pyridine-3-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-2-[[4-[(methylphenylamino)sulfonyl]benzoyl]amino]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2004:681500 CAPLUS DOCUMENT NUMBER: 141:195212 TITLE: Pharmaceutics

INVENTOR (S):

141:195321
Pharmaceutical compositions comprising thieno[2,3-c]pyridines
Gregor, Pauly Harris, Nicholas; Koppel, Juraj; Zhuk, Regina
Rimonyx Pharmaceuticals Ltd., Israel
PCT Int. Appl., 87 pp.
CODEN: PIXXD2
Patent

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent English 1

PATENT NO.		APPLICATION NO.	
WO 2004069149 WO 2004069149	A2 20040819	WO 2004-IL121	
		BA, BB, BG, BR, BW,	BY, BZ, CA, CH,
CN, CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KP, KR, KZ, LC,
LK, LR, LS,	LT, LU, LV, MA,	MD, MG, MK, MN, MW,	MX, MZ, NA, NI
		SD, SL, SZ, TZ, UG,	
BG, CH, CY,	. CZ, DE, DK, EE,	ES, FI, FR, GB, GR,	HU, IE, IT, LU,
		TR, BF, BJ, CF, CG,	CI, CM, GA, GN,
	MR, NE, SN, TD,		
		AU 2004-210241	
		CA 2004-2515102	
EP 1589970	A2 20051102	EP 2004-708427	20040205
		GB, GR, IT, LI, LU,	
		CY, AL, TR, BG, CZ,	EE, HU, SK
CN 1771037	A 20060510	CN 2004-80009369	
JP 2006516610	T 20060706	JP 2006-502633	20040205
		IN 2005-DN3405	
MX 2005PA08397	A 20060217	MX 2005-PA8397	20050805
US 2006135529	A1 20060622	US 2005-543065	20051019
PRIORITY APPLN. INFO.:		IL 2003-154306	A 20030205
		WO 2004-IL121	¥ 20040205
OTHER SOURCE(S):		21	

R SOURCE(S): MARPAT 141:195321
The present invention provides thieno[2,3-c]pyridines, and pharmaceutical compns. comprising thieno[2,3-c]pyridines. The compds. capable of inhibiting glycosaminoglycan (GAG) interactions with effector cell adhesion mols. (ECAM) are useful for treating diseases and disorders mediated by GAG-ECAMs interactions, particularly inflammatory and autoimmune diseases, viral diseases, cancer, and amyloid disorders. Thus, a capsule contained a thieno[2,3-c]pyridine 40.0, starch 109.0, and Mg stearate 1.0 mg.
533904-03-9P 738620-45-6P
BL: PAC (Pharmacological activity), SPN (Synthetic preparation); THU

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(pharmaceutical compns. comprising thieno[2,3-c]pyridines)

Figure 2-2 CAPLUS Computer Com

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

738620-45-6 CAPLUS

Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-2-[[4-[4-methyl-1-piperazinyl)sulfonyl]benzoyl]amino]- (CA INDEX NAME)

0

440334-81-6 449767-27-5 449767-88-8
449767-89-9 449768-16-5 449768-37-0
449768-18-8 449768-33-0 449768-67-6
449768-77-8 449768-93-0 449768-67-6
449768-77-8 449768-93-6 449783-27-1
486453-17-2 496453-18-3 486453-16-1
486453-17-2 496453-22-9 466453-24-1
486453-25-2 496453-26-3 486453-24-1
486453-25-2 496453-26-3 486453-24-1
486453-25-2 489470-30-6 489470-31-4
489470-38-6 489471-00-3 489470-10-4
489471-35-2 489471-00-3 489471-01-4
489471-25-2 489471-29-6 489471-31-0
489471-37-4 489471-39-6 2499471-31-0
489471-37-4 489471-39-6 2499471-31-0
489471-35-4 681264-20-6 681439-14-5
681439-15-6 738620-43-4 738620-44-5
738620-48-9 738620-43-4 738620-44-5
738620-48-9 738620-43-4 738620-44-5
738620-48-9 738620-43-6 738620-50-3
RL: PRC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. comprising thieno[2,3-c]pyridines)
440334-81-6 CAPLUS
Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[(4-[(diethylamino)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-, ethyl ester (CA INDEX NAME)

RN 449767-27-5 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 4,5,6,7-tetrahydro-6-methyl-2-[[4[(1,3,3-trimethyl-6-azabicyclo[3.2.1]oct-6-yl)sulfonyl]benzoyl]amino](CA INDEX NAME)

RN 449767-88-8 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-6-ethy1-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-y1]-4-[(diethylamino)sulfony1]- (CA INDEX NAME)

RN 449767-89-9 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(butylethylamino)sulfonyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

$$i^{-Pr} \xrightarrow{S} \underbrace{NH^{-}C^{-}NH_{2}}^{S} \xrightarrow{BL} \underbrace{S}^{RL}$$

RN 449768-53-0 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 4,5,6,7-tetrahydro-6-(1-methylethyl)2-[[4-[(methyl-phenylamino] sulfonyl]benzoyl]amino] (CA INDEX NAME)

RN 449768-67-6 CAPLUS

Thieno(2,3-c)pyridine-3-carboxamide, 2-[[4-[(3,5-dimethyl-1-piperidinyl)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-(CA INDEX NAME)

RN 449768-77-8 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-2(1H)-isoquinolinyl)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-(CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 449768-16-5 CAPLUS

Thieno(2,3-c]pyridine-3-carboxylic acid, 2-[(4([but/methylamino]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1methylethyl)-, ethyl ester (CA INDEX NAME)

RN 449768-37-0 CAPLUS

Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[3,4-dihydro-1(2H)-quinolinyl)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-, ethyl ester (CA INDEX NAME)

RN 449768-51-8 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(butylethylamino)sulfonyl]benz
oyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 449768-83-6 CAPLUS

Banzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CA INDEX NAME)

RN 449783-27-1 CAPLUS

Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[[hexahydro-1H-azepin-1-yl]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-, ethylester (CA INDEX NAME)

RN 486453-13-8 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CA INDEX NAME)

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RN 486453-14-9 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(dipropylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-16-1 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(dibutylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-17-2 CAPLUS
CN Benzamide, N-{3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yll-4-[[butylmethylamino]sulfonyl]- (CA INDEX NAME)

14 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 486453-22-9 CAPLUS

Senzamido, N-[3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pycidin-2-yl]-4-{1-piperidinylsulfonyl}- (CA INDEX NAME)

RN 486453-24-1 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(3-methyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)

RN 486453-25-2 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(4-methyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)

RN 486453-18-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(butylethylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-20-7 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(di-2-propenylamino)sulfonyl]- (9CI) (CA INDEX NAME)

RN 486453-21-8 CAPLUS

Senzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyrdidin-2-yl]-4-(1-pyrcolidinylsulfonyl)- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 486453-26-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(3,5-dimethyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)

RN 486453-27-4 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-(4-morpholinylsulfony1)- (CA INDEX NAME)

RN 486453-29-6 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c)pyridin-2-y1]-4-[[bis(2-methoxyethy1)amino]sulfony1]- (CA INDEX NAME)

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- RN 489470-30-6 CAPLUS
 CN Benzamide, N-[3-(2-benzothiazoly1)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(dipropylamino)sulfonyl]- (CA INDEX NAME)
- Et NH-C O
- RN 489470-38-4 CAPLUS
 CN Benzamide, N-{3-(2-benzothiazolyl)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c)pyridin-2-yl]-4-{(di-2-propenylamino)sulfonyl]- (9CI) (CA INDEX NAME)
- Et NH-C CH2-CH=-CH2
- RN 489470-54-4 CAPLUS
 CN Benzamide, N-[3-(2-benzothiazoly1)-6-ethy1-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(hewahydro-IH-azepin-1-yl)sulfonyl]- (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
- 1-Pr NH-C- S NH-C- CH2-CH= CH2
- RN 489471-00-3 CAPLUS
 CN Benzamide, N-(3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-(1-piperidinylsulfonyl)- (CA INDEX NAME)
- i-Pr NH-C S NH-C
- RN 489471-01-4 CAPLUS

 Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-[(2-methyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)
- 1-Pr NH-C
- RN 489471-04-7 CAPLUS CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-(1-

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

- RN 489470-89-5 CAPLUS

 Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[[4-(ethoxycarbonyl)-1-piperazinyl]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-, ethyl ester (CA INDEX NAME)
- i-Pr NH-C-OEt
- RN 489470-97-5 CAPLUS
 CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylathyl)thieno[2,3-c]pyridin-2-yl]-4-{(butylethylamino)sulfonyl}- (CA INDEX NAME)
- 1-Pr NH-C 0 Et | S-N-Bu-n
- RN 489470-98-6 CAPLUS

 CN Benzamide, N-[3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-{1-methylethyllthieno[2,3-c]pyridin-2-yl]-4-{(di-2-propenylamino)sulfonyl]-(9CI) (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) methylethyl)thieno[2,3-c]pyridin-2-yl]-4-(4-morpholinylaulfonyl)- (CAINOEX NAME)
- 1-Pr NH-C S NH-C S
- RN 489471-11-6 CAPLUS

 Thieno(2,3-c]pyridine-6(5H)-carboxylic acid, 3-(2-benzothiazolyl)-2-[[4[(dicthylamino) sulfonyl]benzoyl]amino]-4,7-dihydro-, ethyl ester (CA
 INDEX NAME)
- Eto-C NHH-C NEt2
- RN 489471-16-1 CAPLUS

 Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[(di-2-propenylamino) sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-, methyl ester (9CI) (CA INDEX NAME)
- Me Me O O CH2-CH= CH2

 HN S NH-C O O CH2-CH= CH2

 Me Me C-OMe
- RN 489471-25-2 CAPLUS
 CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl
]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME) *

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RN 489471-29-6 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-{[butylmethylamino]sulfonyi]ben zoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

RN 489471-31-0 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(cyclohexylmethylamino)sulfony
l]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

RN 489471-38-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[4-[[[3-(aminocarbonyl)-4,5,6,7-tetrahydro-5,5,7,7-tetramethylthieno[2,3-c]pyridin-2-yl]amino]carbonyl]phenyl]sulfony
1]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 524706-73-8 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(1,3,3-trimethyl-6-azabicyclo[3.2.1]oct-6-yl)sulfonyl]-(CA INDEX NAME)

RN 533895-61-3 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-1(2H)-quinolinyl)sulfonyl]benzoyl]amino]-6-ethyl-4,5,6,7-tetrahydro-N-methyl-(CA INDEX NAME)

RN 533904-54-0 CAPLUS CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl

Me Me S NH-C-OEt

RN 489471-39-8 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-1(2H)-quinolinyl)sulfonyl]benzoyl}amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-(CA INDEX NAME)

RN 524694-99-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6(phenylmethyl)thieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CA
INDEX NAME)

RN 524695-12-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(methylphenylamino)sulfonyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) | amino] -6-ethyl-4,5,6,7-tetrahydro-N-methyl- (CA INDEX NAME)

RN 681264-20-0 CAPLUS
CN Benzanide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-5,5,7,7-tetramethylthieno[2,3-c]pyridin-2-yl]-4-[(3,4-dihydro-1(2H)-quinolinyl)sulfonyl)- (CA INDEX NAME)

RN 681439-14-5 CAPLUS

Thieno(2,3-c)pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-2(1H)-isoquinolinyl) sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- [CA INDEX NAME)

RN 681439-15-6 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[[bis(2-

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) methoxyethyl) amino] sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

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738620-43-4 CAPLUS
1-Piperazinecarboxylic acid, 4-[[4-[[[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]amino]carbonyl]phenyl]sulfony
1]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

738620-44-5 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-2-[[4[[ethyl:phenyl:methyl]amino]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro(CA INDEX NAME)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

738620-48-9 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-methyl-2[[4-[(4-methyl-1-piperazinyl)sulfonyl]benzoyl]amino]- (CA INDEX NAME)

(Continued)

738620-49-0 CAPLUS Benzamide, N-(3-(2-benzothiazoly1)-6-ethy1-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-y1]-4-[(4-methyl-1-piperaziny1)sulfony1]-, monohydrochloride (SCI) (CA INDEX NAME)

• HC1

738620-50-3 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl
]amino]-6-ethyl-4,5,6,7-tetrahydro-N-4-morpholinyl- (CA INDEX NAME)

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:826913 CAPLUS
DOCUMENT NUMBER: 139:49321
TITLE: Property-based design of GPCR-targeted library
Balakin, Konstantin V.; Tkachenko, Sergey E.; Lang,
Stanley A.; Okun, Ilya; Ivashchenko, Andrey A.;
Savchuk, Nikolay P.
CORPORATE SOURCE: Chemical Diversity Labs Inc., San Diego, CA, 92121,
USA
SOURCE: Journal of Chemical Information and Computer Sciences
(2002), 42(6), 1332-1342
CODEN; JCISDB; ISSN: 0055-2338
PUBLISHER: American Chemical Society
Journal
LANGUAGE: English
AB The design of a GPCR-targeted library, based on a scoring scheme for the
classification of moils. into "GPCR-ligand-like", is outlined. The methodol. is a valuable tool that can add in the
selection and prioritization of potential GPCR ligands for bioscreening
from large collections of compds. It is based on the distillation of
knowledge
from large databases of GPCR and non-GPCR active agents. The method
employed a set of descriptors for encoding the mol. structures and by
training of a neural network for classifying the mols. The mol.
requirements were profiled and validated by using available databases of
GPCR- and non-GPCR-active agents. The method enables efficient
qualification or disqualification of a mol. as a potential GPCR ligand and
represents a useful tool for constraining the size of GPCR-active
drugs.

IT 478932-86-4

libraries that will help speed up the development of new GPCR-active drugs.

478932-86-4

EL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(property-based design of GPCR-targeted library)

478932-86-4 CAPLUS

Thieno[2,3-c]pyridine-3-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-2-[[4-[(4,6,6-trimethyl-2-azabicyclo[2.2.1]hept-2-yl)sulfonyl]benzoyl]amino]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 22

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(FILE 'HOME' ENTERED AT 11:14:33 ON 12 DEC 2007)

FILE 'REGISTRY' ENTERED AT 11:14:43 ON 12 DEC 2007

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 3524 S L1 FULL

FILE 'CAPLUS' ENTERED AT 11:15:11 ON 12 DEC 2007

L4 3 S L3 FULL

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